

Database :        Issued\_Patents\_AA:\*

- 1: /cgn2\_6/ptodata/2/iaa/5A\_COMB.pep:\*
- 2: /cgn2\_6/ptodata/2/iaa/5B\_COMB.pep:\*
- 3: /cgn2\_6/ptodata/2/iaa/6A\_COMB.pep:\*
- 4: /cgn2\_6/ptodata/2/iaa/6B\_COMB.pep:\*
- 5: /cgn2\_6/ptodata/2/iaa/PCTUS\_COMB.pep:\*
- 6: /cgn2\_6/ptodata/2/iaa/backfiles1.pep:\*

Pred. No. is the number of results predicted by chance to have a score greater than or equal to the score of the result being printed, and is derived by analysis of the total score distribution.

#### SUMMARIES

Result		%	Query				
No.	Score	Match	Length	DB	ID	Description	
1	1771	100.0	331	3	US-09-413-231-1	Sequence 1, Appli	
2	1771	100.0	331	3	US-09-413-231-2	Sequence 2, Appli	
3	1771	100.0	331	3	US-09-413-231-3	Sequence 3, Appli	
4	1473	83.2	331	3	US-09-413-231-4	Sequence 4, Appli	
5	1363.5	77.0	338	3	US-09-413-231-7	Sequence 7, Appli	
6	1355.5	76.5	338	3	US-09-413-231-6	Sequence 6, Appli	
7	991.5	56.0	329	3	US-09-413-231-5	Sequence 5, Appli	
8	991.5	56.0	329	3	US-09-413-231-9	Sequence 9, Appli	
9	985.5	55.6	333	3	US-09-413-231-10	Sequence 10, Appl	
10	743.5	42.0	321	3	US-09-413-231-8	Sequence 8, Appli	
11	540	30.5	188	3	US-08-861-774E-16	Sequence 16, Appl	
12	336	19.0	390	4	US-09-252-991A-20513	Sequence 20513, A	
13	303	17.1	344	4	US-09-252-991A-28503	Sequence 28503, A	
14	290	16.4	360	4	US-09-489-039A-9976	Sequence 9976, Ap	
15	233	13.2	386	2	US-08-553-367A-2	Sequence 2, Appli	
16	233	13.2	386	3	US-09-295-306-2	Sequence 2, Appli	

Database : SPTREMBL\_25:\*

- 1: sp\_archaea:\*
- 2: sp\_bacteria:\*
- 3: sp\_fungi:\*
- 4: sp\_human:\*
- 5: sp\_invertebrate:\*
- 6: sp\_mammal:\*
- 7: sp\_mhc:\*
- 8: sp\_organelle:\*
- 9: sp\_phage:\*
- 10: sp\_plant:\*
- 11: sp\_rodent:\*
- 12: sp\_virus:\*
- 13: sp\_vertebrate:\*
- 14: sp\_unclassified:\*
- 15: sp\_rvirus:\*
- 16: sp\_bacteriaphage:\*
- 17: sp\_archaeophages:\*

Pred. No. is the number of results predicted by chance to have a score greater than or equal to the score of the result being printed, and is derived by analysis of the total score distribution.

#### SUMMARIES

Result No.	Score	% Query		DB	ID	Description
		Match	Length			
1	1308	73.9	331	3	Q9C1G1	Q9c1g1 kallichroma
2	1015.5	57.3	331	2	Q9LCZ2	Q9lcz2 streptomyce
3	1005.5	56.8	329	2	Q9ANU0	Q9anu0 streptomyce
4	843.5	47.6	262	2	Q9FAB6	Q9fab6 streptomyce
5	837.5	47.3	262	2	Q9FAC2	Q9fac2 streptomyce
6	830.5	46.9	262	2	Q9FAB8	Q9fab8 streptomyce
7	825.5	46.6	262	2	Q9FAC1	Q9fac1 streptomyce
8	823.5	46.5	262	2	Q9FAB9	Q9fab9 streptomyce
9	822.5	46.4	262	2	Q9FAC0	Q9fac0 streptomyce
10	819.5	46.3	262	2	Q9FAC3	Q9fac3 streptomyce
11	800.5	45.2	262	2	Q9FAB7	Q9fab7 streptomyce
12	685.5	38.7	221	2	Q9F5K9	Q9f5k9 streptomyce
13	405	22.9	237	2	Q9X6N2	Q9x6n2 streptomyce

Database : SwissProt\_42:\*

Pred. No. is the number of results predicted by chance to have a score greater than or equal to the score of the result being printed, and is derived by analysis of the total score distribution.

# SUMMARIES

Result No.	Score	% Query		DB	ID	Description
		Match	Length			
1	1766	99.7	331	1	IPNS_EMENI	P05326 emericella
2	1468	82.9	331	1	IPNS_PENCH	P08703 penicillium
3	1350.5	76.3	338	1	IPNS_CEPAC	P05189 cephalospor
4	1041	58.8	328	1	IPNS_NOCLA	P27744 nocardia la
5	1014.5	57.3	329	1	IPNS_STRJU	P18286 streptomyce
6	993.5	56.1	326	1	IPNS_LYSLA	Q48739 lysobacter
7	986.5	55.7	329	1	IPNS_STRCL	P10621 streptomyce
8	985.5	55.6	326	1	IPNS_FLASS	P16020 flavobacter
9	985.5	55.6	329	1	IPNS_STRGR	Q54243 streptomyce
10	980.5	55.4	333	1	IPNS_STRLP	P12438 streptomyce
11	738.5	41.7	321	1	IPNS_STRCT	Q53932 streptomyce
12	218	12.3	291	1	FLS_MATIN	O04395 matthiola i
13	218	12.3	397	1	ISP7_SCHPO	P40902 schizosacch
14	192.5	10.9	349	1	FLS_SOLTU	Q41452 solanum tub
15	189	10.7	334	1	FLS_EUSGR	Q9m547 eustoma gra
16	188	10.6	335	1	FLS_CITUN	Q9zwq9 citrus unsh
17	187	10.6	348	1	FLS_PETHY	Q07512 petunia hyb
18	184.5	10.4	369	1	FL3H_PETHY	Q07353 petunia hyb
19	183.5	10.4	337	1	FLS_MALDO	Q9xhg2 malus domes
20	177	10.0	356	1	FL3H_CALCH	Q05963 callistephu
21	176.5	10.0	318	1	ACCO_DIOKA	Q8s932 diospyros k

Database :       PIR\_78:\*  
               1:  pir1:\*  
               2:  pir2:\*  
               3:  pir3:\*  
               4:  pir4:\*

Pred. No. is the number of results predicted by chance to have a score greater than or equal to the score of the result being printed, and is derived by analysis of the total score distribution.

# SUMMARIES

Result No.	Score	% Query		Length	DB	ID	Description
		Match					
1	1766	99.7		331	2	A27355	isopenicillin N sy
2	1476	83.3		331	2	S04441	isopenicillin N sy
3	1468	82.9		331	2	A26467	isopenicillin N sy
4	1350.5	76.3		338	2	S09312	isopenicillin N sy
5	1350.5	76.3		338	2	A24567	isopenicillin N sy
6	1041	58.8		328	2	S15284	isopenicillin N sy
7	993.5	56.1		326	2	S54099	isopenicillin N sy
8	986.5	55.7		329	2	A29894	isopenicillin N sy
9	985.5	55.6		326	2	S08218	isopenicillin N sy
10	985.5	55.6		329	2	A61155	isopenicillin N sy
11	980.5	55.4		333	2	B32344	isopenicillin N sy
12	738.5	41.7		321	2	A58458	isopenicillin N sy
13	335	18.9		334	2	E83122	probable iron/asco
14	303	17.1		320	2	C83628	probable oxidoredu
15	246.5	13.9		329	2	G86472	probable hyoscyami
16	241	13.6		306	2	T45586	hypothetical prote
17	233	13.2		386	2	T09664	gibberellin 20-oxi

Database : Published\_Applications\_AA:\*

- 1: /cgn2\_6/ptodata/2/pubpaa/US07\_PUBCOMB.pep:\*
- 2: /cgn2\_6/ptodata/2/pubpaa/PCT\_NEW\_PUB.pep:\*
- 3: /cgn2\_6/ptodata/2/pubpaa/US06\_NEW\_PUB.pep:\*
- 4: /cgn2\_6/ptodata/2/pubpaa/US06\_PUBCOMB.pep:\*
- 5: /cgn2\_6/ptodata/2/pubpaa/US07\_NEW\_PUB.pep:\*
- 6: /cgn2\_6/ptodata/2/pubpaa/PCTUS\_PUBCOMB.pep:\*
- 7: /cgn2\_6/ptodata/2/pubpaa/US08\_NEW\_PUB.pep:\*
- 8: /cgn2\_6/ptodata/2/pubpaa/US08\_PUBCOMB.pep:\*
- 9: /cgn2\_6/ptodata/2/pubpaa/US09A\_PUBCOMB.pep:\*
- 10: /cgn2\_6/ptodata/2/pubpaa/US09B\_PUBCOMB.pep:\*
- 11: /cgn2\_6/ptodata/2/pubpaa/US09C\_PUBCOMB.pep:\*
- 12: /cgn2\_6/ptodata/2/pubpaa/US09\_NEW\_PUB.pep:\*
- 13: /cgn2\_6/ptodata/2/pubpaa/US10A\_PUBCOMB.pep:\*
- 14: /cgn2\_6/ptodata/2/pubpaa/US10B\_PUBCOMB.pep:\*
- 15: /cgn2\_6/ptodata/2/pubpaa/US10C\_PUBCOMB.pep:\*
- 16: /cgn2\_6/ptodata/2/pubpaa/US10\_NEW\_PUB.pep:\*
- 17: /cgn2\_6/ptodata/2/pubpaa/US60\_NEW\_PUB.pep:\*
- 18: /cgn2\_6/ptodata/2/pubpaa/US60\_PUBCOMB.pep:\*

Pred. No. is the number of results predicted by chance to have a score greater than or equal to the score of the result being printed, and is derived by analysis of the total score distribution.

#### SUMMARIES

RESULTS							
Result No.	Score	%		Length	DB	ID	Description
		Query	Match				
1	1771	100.0	331	9	US-09-924-841-1	Sequence 1, Appli	
2	1771	100.0	331	9	US-09-924-841-2	Sequence 2, Appli	
3	1771	100.0	331	9	US-09-924-841-3	Sequence 3, Appli	
4	1754	99.0	331	15	US-10-369-493-13125	Sequence 13125, A	
5	1473	83.2	331	9	US-09-924-841-4	Sequence 4, Appli	
6	1363.5	77.0	338	9	US-09-924-841-7	Sequence 7, Appli	
7	1355.5	76.5	338	9	US-09-924-841-6	Sequence 6, Appli	
8	991.5	56.0	329	9	US-09-924-841-5	Sequence 5, Appli	
9	991.5	56.0	329	9	US-09-924-841-9	Sequence 9, Appli	
10	985.5	55.6	333	9	US-09-924-841-10	Sequence 10, Appl	
11	743.5	42.0	321	9	US-09-924-841-8	Sequence 8, Appli	
12	540	30.5	188	9	US-09-924-256A-16	Sequence 16, Appl	
13	314.5	17.8	320	15	US-10-369-493-14020	Sequence 14020, A	
14	312.5	17.6	296	15	US-10-369-493-7385	Sequence 7385, Ap	
15	312.5	17.6	306	15	US-10-369-493-4627	Sequence 4627, Ap	
16	270.5	15.3	309	15	US-10-369-493-7649	Sequence 7649, Ap	
17	270.5	15.3	317	15	US-10-369-493-4891	Sequence 4891, Ap	
18	269	15.2	352	16	US-10-437-963-173894	Sequence 173894,	
19	263.5	14.9	340	12	US-10-424-599-179169	Seq	

RESULT 1

IPNS\_EMENI

ID IPNS\_EMENI STANDARD; PRT; 331 AA.  
AC P05326;  
DT 01-NOV-1988 (Rel. 09, Created)  
DT 01-NOV-1988 (Rel. 09, Last sequence update)  
DT 10-OCT-2003 (Rel. 42, Last annotation update)  
DE Isopenicillin N synthetase (EC 1.21.3.1) (IPNS) (Isopenicillin N  
DE synthase).  
GN IPNA OR IPS.  
OS Emericella nidulans (Aspergillus nidulans).  
OC Eukaryota; Fungi; Ascomycota; Pezizomycotina; Eurotiomycetes;  
OC Eurotiales; Trichocomaceae; Emericella.  
OX NCBI\_TaxID=162425;  
RN [1]  
RP SEQUENCE FROM N.A.  
RX MEDLINE=88084424; PubMed=3319778;  
RA Ramon D., Carramolino L., Patino C., Sanchez F., Penalva M.A.;  
RT "Cloning and characterization of the isopenicillin N synthetase gene  
RT mediating the formation of the beta-lactam ring in Aspergillus  
RT nidulans.";  
RL Gene 57:171-181(1987).  
RN [2]  
RP SEQUENCE FROM N.A.  
RX MEDLINE=88314868; PubMed=3045077;  
RA Weigel B.J., Burgett S.G., Chen V.J., Skatrud P.L., Frolik C.A.,  
RA Queener S.W., Ingolia T.D.;  
RT "Cloning and expression in Escherichia coli of isopenicillin N  
RT synthetase genes from Streptomyces lipmanii and Aspergillus  
RT nidulans.";  
RL J. Bacteriol. 170:3817-3826(1988).  
RN [3]  
RP CRYSTALLIZATION.  
RX MEDLINE=95392381; PubMed=7663335;  
RA Roach P.L., Schofield C.J., Baldwin J.E., Clifton I.J., Hajdu J.;  
RT "Crystallization and preliminary X-ray diffraction studies on  
RT recombinant isopenicillin N synthase from Aspergillus nidulans.";  
RL Protein Sci. 4:1007-1009(1995).  
RN [4]  
RP X-RAY CRYSTALLOGRAPHY (2.5 ANGSTROMS).  
RX MEDLINE=95312111; PubMed=7791906;  
RA Roach P.L., Clifton I.J., Fueloep V., Harlos K., Barton G.J.,  
RA Hajdu J., Andersson I., Schofield C.J., Baldwin J.E.;  
RT "Crystal structure of isopenicillin N synthase is the first from a  
RT new structural family of enzymes.";  
RL Nature 375:700-704(1995).  
RN [5]  
RP X-RAY CRYSTALLOGRAPHY (1.45 ANGSTROMS).  
RX MEDLINE=97337872; PubMed=9194566;  
RA Roach P.L., Clifton I.J., Hensgens C.M., Shibata N., Schofield C.J.,  
RA Hajdu J., Baldwin J.E.;  
RT "Structure of isopenicillin N synthase complexed with substrate and  
RT the mechanism of penicillin formation.";  
RL Nature 387:827-830(1997).  
RN [6]  
RP X-RAY CRYSTALLOGRAPHY (1.35 ANGSTROMS).  
RX MEDLINE=20005505; PubMed=10537113;

RA Burzlaff N.I., Rutledge P.J., Clifton I.J., Hensgens C.M.H.,  
 RA Pickford M., Adlington R.M., Roach P.L., Baldwin J.E.;  
 RT "The reaction cycle of isopenicillin N synthase observed by X-ray  
 RT diffraction.";  
 RL Nature 401:721-724(1999).  
 RN [7]  
 RP X-RAY CRYSTALLOGRAPHY (1.3 ANGSTROMS).  
 RX MEDLINE=21628900; PubMed=11755401;  
 RA Ogle J.M., Clifton I.J., Rutledge P.J., Elkins J.M., Burzlaff N.I.,  
 RA Adlington R.M., Roach P.L., Baldwin J.E.;  
 RT "Alternative oxidation by isopenicillin N synthase observed by X-ray  
 RT diffraction.";  
 RL Chem. Biol. 8:1231-1237(2001).  
 CC -!- FUNCTION: Removes, in the presence of oxygen, 4 hydrogen atoms  
 CC from delta-L-(alpha-aminoadipyl)-L-cysteinyl-D-valine (ACV) to  
 CC form the azetidinone and thiazolidine rings of isopenicillin.  
 CC -!- CATALYTIC ACTIVITY: N-[(5S)-5-amino-5-carboxypentanoyl]-L-  
 CC cysteinyl-D-valine + O(2) = isopenicillin N + 2 H(2)O.  
 CC -!- COFACTOR: Iron and ascorbate.  
 CC -!- PATHWAY: Biosynthesis of penicillin and cephalosporin.  
 CC -!- SIMILARITY: Belongs to the iron/ascorbate-dependent oxidoreductase  
 CC family.  
 CC -----  
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 DR EMBL; M18111; AAA33311.1; -.  
 DR EMBL; M21882; AAA33310.1; -.  
 DR EMBL; A10846; CAA00924.1; -.  
 DR PIR; A27355; A27355.  
 DR PDB; 1IPS; 25-MAR-98.  
 DR PDB; 1BK0; 13-JAN-99.  
 DR PDB; 1BLZ; 13-JAN-99.  
 DR PDB; 1QIQ; 16-JUN-00.  
 DR PDB; 1QJE; 29-JUN-00.  
 DR PDB; 1QJF; 29-JUN-00.  
 DR PDB; 1HB1; 17-JAN-02.  
 DR PDB; 1HB2; 17-JAN-02.  
 DR PDB; 1HB3; 17-JAN-02.  
 DR PDB; 1HB4; 17-JAN-02.  
 DR InterPro; IPR005123; 2OG-FeII\_Oxy.  
 DR InterPro; IPR002283; IPN\_synth.  
 DR InterPro; IPR002057; Isopen\_N\_synth.  
 DR Pfam; PF03171; 2OG-FeII\_Oxy; 1.  
 DR PRINTS; PR00682; IPNSYNTHASE.  
 DR PROSITE; PS00185; IPNS\_1; 1.  
 DR PROSITE; PS00186; IPNS\_2; 1.  
 KW Antibiotic biosynthesis; Oxidoreductase; Iron; Vitamin C;  
 KW 3D-structure.  
 FT METAL 214 214 IRON.  
 FT METAL 216 216 IRON.  
 FT METAL 270 270 IRON.

FT	STRAND	6	6
FT	STRAND	11	13
FT	HELIX	15	18
FT	HELIX	22	37
FT	TURN	38	39
FT	STRAND	41	45
FT	HELIX	51	64
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FT	STRAND	74	74
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FT	STRAND	94	94
FT	TURN	95	97
FT	STRAND	98	98
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FT	TURN	108	109
FT	TURN	112	113
FT	HELIX	115	118
FT	TURN	119	120
FT	TURN	122	123
FT	TURN	132	134
FT	TURN	136	137
FT	HELIX	138	163
FT	TURN	164	165
FT	TURN	168	171
FT	HELIX	172	174
FT	TURN	177	179
FT	STRAND	183	189
FT	HELIX	197	199
FT	STRAND	201	202
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FT	STRAND	238	241
FT	TURN	246	247
FT	STRAND	249	253
FT	HELIX	255	260
FT	TURN	261	263
FT	STRAND	270	273
FT	STRAND	279	286
FT	TURN	290	291
FT	STRAND	293	293
FT	TURN	299	300
FT	TURN	302	303
FT	STRAND	312	312
FT	HELIX	313	328

SQ SEQUENCE 331 AA; 37522 MW; 5BA1A726E9EEFA25 CRC64;

Query Match 99.7%; Score 1766; DB 1; Length 331;

Best Local Similarity 99.7%; Pred. No. 2.7e-143;

Matches 330; Conservative 0; Mismatches 1; Indels 0; Gaps 0;

QY 1 MGSVSKANVPKIDVSPLFGDDQAAKMRVAQQIDAASRDTGFFYAVNHGINVQRLSQKTKE 60



Db	1		MGSVSKANVPKIDVSPLFGDDQAAKMRVAQQIDAASRDTGFFYAVNHGINVQRLSQKTKE	60
Qy	61		FHMSITPEEKWDLAIRAYNKEHQDQVRAGYYLSIPGKKAVESFCYLNPNFTPDHPRIQAK	120
Db	61		FHMSITPEEKWDLAIRAYNKEHQDQVRAGYYLSIPGKKAVESFCYLNPNFTPDHPRIQAK	120
Qy	121		TPTHEVNVWPDETKHPGFQDFAEQYYWDVFLSSALLKGYALALGKEENFFARHFKPDDT	180
Db	121		TPTHEVNVWPDETKHPGFQDFAEQYYWDVFLSSALLKGYALALGKEENFFARHFKPDDT	180
Qy	181		LASVVLIRYPYLDPYPEAAIKTAADGTKLSFRWHEDVSLITVLYQSNVQNLQVETAAGYQ	240
Db	181		LASVVLIRYPYLDPYPEAAIKTAADGTKLSFEWHEDVSLITVLYQSNVQNLQVETAAGYQ	240
Qy	241	25 26 	DIEADDTGYLINC <sup>25</sup> GSYMAHL <sup>26</sup> TNNYYKAPIHRVKWVNAERQSLPFFVNLGYDSVIDPFDPR	300
Db	241		DIEADDTGYLINC <sup>25</sup> GSYMAHL <sup>26</sup> TNNYYKAPIHRVKWVNAERQSLPFFVNLGYDSVIDPFDPR	300
Qy	301	268 270 	EPNGKSDREPLSYGDYLNGLVSLINKNGQT	331
Db	301		EPNGKSDREPLSYGDYLNGLVSLINKNGQT	331

RESULT 2

IPNS\_PENCH

ID IPNS\_PENCH STANDARD; PRT; 331 AA.  
 AC P08703;  
 DT 01-JAN-1988 (Rel. 06, Created)  
 DT 01-JAN-1988 (Rel. 06, Last sequence update)  
 DT 10-OCT-2003 (Rel. 42, Last annotation update)  
 DE Isopenicillin N synthetase (EC 1.21.3.1) (IPNS) (Isopenicillin N  
 DE synthase).  
 GN PCBC OR IPS.  
 OS Penicillium chrysogenum.  
 OC Eukaryota; Fungi; Ascomycota; Pezizomycotina; Eurotiomycetes;  
 OC Eurotiales; Trichocomaceae; mitosporic Trichocomaceae; Penicillium.  
 OX NCBI\_TaxID=5076;  
 RN [1]  
 RP SEQUENCE FROM N.A.  
 RC STRAIN=23X-80-269-37-2;  
 RX MEDLINE=87163529; PubMed=3104145;  
 RA Carr L.G., Skatrud P.L., Scheetz M.E. II, Queener S.W., Ingolia T.D.;  
 RT "Cloning and expression of the isopenicillin N synthetase gene from  
 RT Penicillium chrysogenum."  
 RL Gene 48:257-266(1986).

RN [2]  
 RP SEQUENCE FROM N.A.  
 RC STRAIN=AS-P-78;  
 RX MEDLINE=89281495; PubMed=2499766;  
 RA Barrredo J.L., Cantoral J.M., Alvarez E., Diez B., Martin J.F.;  
 RT "Cloning, sequence analysis and transcriptional study of the  
 RT isopenicillin N synthase of Penicillium chrysogenum AS-P-78."  
 RL Mol. Gen. Genet. 216:91-98(1989).  
 CC -!- FUNCTION: Removes, in the presence of oxygen, 4 hydrogen atoms  
 CC from delta-L-(alpha-aminoadipyl)-L-cysteinyl-D-valine (ACV) to  
 CC form the azetidinone and thiazolidine rings of isopenicillin.  
 CC -!- CATALYTIC ACTIVITY: N-[(5S)-5-amino-5-carboxypentanoyl]-L-  
 CC cysteinyl-D-valine + O(2) = isopenicillin N + 2 H(2)O.  
 CC -!- COFACTOR: Iron and ascorbate.  
 CC -!- PATHWAY: Biosynthesis of penicillin and cephalosporin.  
 CC -!- SIMILARITY: Belongs to the iron/ascorbate-dependent oxidoreductase  
 CC family.

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DR EMBL; M15083; AAA33696.1; -.  
 DR EMBL; X17436; CAA35480.1; -.  
 DR PIR; A26467; A26467.  
 DR PIR; S04441; S04441.  
 DR HSSP; P05326; 1BLZ.  
 DR InterPro; IPR005123; 2OG-FeII\_Oxy.  
 DR InterPro; IPR002283; IPN\_synth.  
 DR InterPro; IPR002057; Isopen\_N\_synth.  
 DR Pfam; PF03171; 2OG-FeII\_Oxy; 1.



RESULT 3

IPNS\_CEPAC

ID IPNS\_CEPAC STANDARD; PRT; 338 AA.  
AC P05189; Q00047;  
DT 13-AUG-1987 (Rel. 05, Created)  
DT 13-AUG-1987 (Rel. 05, Last sequence update)  
DT 10-OCT-2003 (Rel. 42, Last annotation update)  
DE Isopenicillin N synthetase (EC 1.21.3.1) (IPNS) (Isopenicillin N  
DE synthase).  
GN PCBC OR IPS.  
OS Cephalosporium acremonium (Acremonium chrysogenum).  
OC Eukaryota; Fungi; Ascomycota; Pezizomycotina; Sordariomycetes;  
OC Hypocreomycetidae; Hypocreales; Hypocreaceae; mitosporic Hypocreaceae;  
OC Acremonium.  
OX NCBI\_TaxID=5044;  
RN [1]  
RP SEQUENCE FROM N.A.  
RX MEDLINE=86040479; PubMed=3903520;  
RA Samson S.N., Belagaje R., Blankenship D.T., Chapman J.L., Perry D.,  
RA Skatrud P.L., Vanfrank R.M., Abraham E.P., Baldwin J.E., Queener S.W.,  
RA Ingolia T.D.;  
RT "Isolation, sequence determination and expression in Escherichia coli  
RT of the isopenicillin N synthetase gene from Cephalosporium  
RT acremonium.";  
RL Nature 318:191-194(1985).  
RN [2]  
RP SEQUENCE FROM N.A.  
RC STRAIN=N-2;  
RX MEDLINE=90152376; PubMed=2620834;  
RA Ramsden M., McQuade B.A., Saunders K., Turner M.K., Harford S.;  
RT "Characterization of a loss-of-function mutation in the isopenicillin  
RT N synthetase gene of Acremonium chrysogenum.";  
RL Gene 85:267-273(1989).  
RN [3]  
RP SEQUENCE OF 3-52.  
RC STRAIN=ATCC 60777;  
RX MEDLINE=85285585; PubMed=3839755;  
RA Baldwin J.E., Gagnon J., Ting H.H.;  
RT "N-terminal amino acid sequence and some properties of  
RT isopenicillin-N synthetase from Cephalosporium acremonium.";  
RL FEBS Lett. 188:253-256(1985).  
RN [4]  
RP SEQUENCE OF 40-78 AND 237-264, AND PHOTOAFFINITY LABELLING.  
RX MEDLINE=90197638; PubMed=2317203;  
RA Baldwin J.E., Coates J.B., Moloney M.G., Pratt A.J., Willis A.C.;  
RT "Photoaffinity labelling of isopenicillin N synthetase.";  
RL Biochem. J. 266:561-567(1990).  
RN [5]  
RP MUTAGENESIS OF HIS-272.  
RX MEDLINE=94357414; PubMed=8076799;  
RA Tiow-Suan S., Tan D.S.;  
RT "Histidine-272 of isopenicillin N synthase of Cephalosporium  
RT acremonium, which is possibly involved in iron binding, is essential  
RT for its catalytic activity.";  
RL FEMS Microbiol. Lett. 120:241-247(1994).  
RN [6]  
RP MUTAGENESIS OF HISTIDINE RESIDUES.

RX MEDLINE=96132822; PubMed=8557701;  
RA Tan D.S., Sim T.S.;  
RT "Functional analysis of conserved histidine residues in Cephalosporium  
RT acremonium isopenicillin N synthase by site-directed mutagenesis.";  
RL J. Biol. Chem. 271:889-894(1996).

RN [7]

RP MUTAGENESIS OF ASP-218.

RX MEDLINE=98079444; PubMed=9418249;

RA Loke P., Sim J., Sim T.S.;

RT "Functional analysis of a conserved aspartate D218 in Cephalosporium  
RT acremonium isopenicillin N synthase.";

RL FEMS Microbiol. Lett. 157:137-140(1997).

RN [8]

RP MUTAGENESIS OF GLN-234.

RX MEDLINE=98369588; PubMed=9703965;

RA Loke P., Sim T.S.;

RT "Catalytic activity in Cephalosporium acremonium isopenicillin N  
RT synthase does not involve glutamine-234.";

RL Biochem. Biophys. Res. Commun. 248:559-561(1998).

RN [9]

RP MUTAGENESIS OF GLUTAMINE RESIDUES.

RX MEDLINE=99045430; PubMed=9826554;

RA Loke P., Sim T.S.;

RT "Analysis of glutamines in catalysis in Cephalosporium acremonium  
RT isopenicillin N synthase by site-directed mutagenesis.";

RL Biochem. Biophys. Res. Commun. 252:472-475(1998).

RN [10]

RP MUTAGENESIS OF HISTIDINE RESIDUES.

RX MEDLINE=98191594; PubMed=9530516;

RA Tan D.S., Ang S.G., Sim T.S.;

RT "Involvement of a third histidine in the ferrous active site of  
RT isopenicillin N synthase of Cephalosporium acremonium repudiated by  
RT recombinant double histidine mutants.";

RL Biochem. Mol. Biol. Int. 44:333-345(1998).

RN [11]

RP MUTAGENESIS OF SER-283.

RX MEDLINE=99006482; PubMed=9841222;

RA Loke P., Sim T.S.;

RT "Mutational evidence for the role of serine-283 in Cephalosporium  
RT acremonium isopenicillin N synthase.";

RL FEMS Microbiol. Lett. 165:353-356(1998).

CC -!- FUNCTION: Removes, in the presence of oxygen, 4 hydrogen atoms  
CC from delta-L-(alpha-aminoadipyl)-L-cysteinyl-D-valine (ACV) to  
CC form the azetidinone and thiazolidine rings of isopenicillin.

CC -!- CATALYTIC ACTIVITY: N-[(5S)-5-amino-5-carboxypentanoyl]-L-  
CC cysteinyl-D-valine + O(2) = isopenicillin N + 2 H(2)O.

CC -!- COFACTOR: Iron and ascorbate.

CC -!- PATHWAY: Biosynthesis of penicillin and cephalosporin.

CC -!- SIMILARITY: Belongs to the iron/ascorbate-dependent oxidoreductase  
CC family.

CC

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CC -----  
DR EMBL; X03148; CAA26927.1; -.  
DR EMBL; M33522; AAA32674.1; -.  
DR PIR; S09312; S09312.  
DR HSSP; P05326; 1BLZ.  
DR InterPro; IPR005123; 2OG-FeII\_Oxy.  
DR InterPro; IPR002283; IPN\_synth.  
DR InterPro; IPR002057; Isopen\_N\_synth.  
DR Pfam; PF03171; 2OG-FeII\_Oxy; 1.  
DR PRINTS; PR00682; IPNSYNTHASE.  
DR PROSITE; PS00185; IPNS\_1; 1.  
DR PROSITE; PS00186; IPNS\_2; 1.  
KW Antibiotic biosynthesis; Oxidoreductase; Iron; Vitamin C.  
FT METAL 216 216 IRON.  
FT METAL 218 218 IRON (BY SIMILARITY).  
FT METAL 272 272 IRON.  
FT SITE 283 283 INVOLVED IN ACV-BINDING.  
FT VARIANT 285 285 P -> L (IN STRAIN N-2; INACTIVE).  
FT MUTAGEN 216 216 H->L: LOSS OF ACTIVITY.  
FT MUTAGEN 218 218 D->L: LOSS OF ACTIVITY.  
FT MUTAGEN 272 272 H->L: LOSS OF ACTIVITY.  
FT CONFLICT 22 22 D -> T (IN REF. 3).  
FT CONFLICT 177 177 S -> F (IN REF. 2).  
SQ SEQUENCE 338 AA; 38433 MW; CFB0B6E27FC04EE9 CRC64;

Query Match 76.3%; Score 1350.5; DB 1; Length 338;  
Best Local Similarity 73.7%; Pred. No. 8.1e-108;  
Matches 249; Conservative 39; Mismatches 43; Indels 7; Gaps 2;

Qy 1 MGS--VSKANVPKIDVSPPLFGDDQAAKMRVAQQIDAASRD TGFFYAVNHGINVQRLSQKT 58  
||| | ||||:|||||||: |: |: ||||| ||||| |||||: ||:|  
Db 1 MGSVPVPVANVPRIDVSPPLFGDDKEKKLEVARAIDAASRD TGFFYAVNHGVDPWLSRET 60  
  
Qy 59 KEFHMSITPEEKWDLAIRAYNKEHQDQVRAGYYLSIPGKKAVESFCYLNPNFTPDHPRIQ 118  
: ||||| |||| ||||| ||||: |: ||||| ||||| |||||: |: |||||:  
Db 61 NKFHMSITDEEKWQLAIRAYNKEHESQIRAGYYLPPIGKKAVESFCYLNPSFSPDHPRIK 120  
  
Qy 119 AKTPTHEVNVWPDETKHPGFQDFAEQYYWDVFG LSSALLKGYALALGKEENFFARHFKPD 178  
|| ||||| ||||: ||: ||||| ||||: |: |||||: |: || ||: |  
Db 121 EPTPMHEVNVWPDEAKHPGFRAFAEKYYWDVFG LSSAVLRGYALALGRDEDFTRHSRRD 180  
  
Qy 179 DTLASVVLIRYPYLDPYEAAIKTAADG TKLSFRWHEDVSLITVLYQSNVQNLQVETAAG 238  
||: ||||| ||||| |||| ||||| ||||| |||||: |||||: |  
Db 181 TTLSSVVLIRYPYLDPYEPAIKTADDG TKLSFEWHEDVSLITVLYQSDVQNLQVKTPOG 240  
  
Qy 239 YQDIEADD TGYLINCGSYMAHLTNYYKAPIHRVKWVNAERQSLPFFVNLGYDSVIDPFD 298  
: ||||: ||||: ||||| ||||: |: || ||||| ||||| |||||: ||: |  
Db 241 WQDIQADD TGFLINCGSYMAHITDDYYPAPIHRVKWVNEERQSLPFFVNLGWEDTIQPWD 300  
  
Qy 299 PR-----EPNGKSDREPLSYGDY LQNGLVSLINKNGQT 331  
| : |: : |||: || || |||||  
Db 301 PATAKDGA KDAKD KPAISYGEYLQGG LRLINKNGQT 338

RESULT 4

IPNS\_NOCLA

ID IPNS\_NOCLA STANDARD; PRT; 328 AA.

AC P27744;

DT 01-AUG-1992 (Rel. 23, Created)

DT 01-AUG-1992 (Rel. 23, Last sequence update)

DT 10-OCT-2003 (Rel. 42, Last annotation update)

DE Isopenicillin N synthetase (EC 1.21.3.1) (IPNS) (Isopenicillin N synthase).

GN PCBC.

OS Nocardia lactamdurans.

OC Bacteria; Actinobacteria; Actinobacteridae; Actinomycetales;

OC Pseudonocardineae; Pseudonocardiaceae; Amycolatopsis.

OX NCBI\_TaxID=1913;

RN [1]

RP SEQUENCE FROM N.A.

RC STRAIN=VAR LC 411;

RX MEDLINE=92065808; PubMed=1956290;

RA Coque J.J.R., Martin J.F., Calzada J.G., Liras P.;

RT "The cephamycin biosynthetic genes pcbAB, encoding a large multidomain peptide synthetase, and pcbC of Nocardia lactamdurans are clustered together in an organization different from the same genes in Acremonium chrysogenum and Penicillium chrysogenum.";

RL Mol. Microbiol. 5:1125-1133(1991).

CC -!- FUNCTION: Removes, in the presence of oxygen, 4 hydrogen atoms from delta-L-(alpha-aminoadipyl)-L-cysteinyl-D-valine (ACV) to form the azetidinone and thiazolidine rings of isopenicillin.

CC -!- CATALYTIC ACTIVITY: N-[(5S)-5-amino-5-carboxypentanoyl]-L-cysteinyl-D-valine + O(2) = isopenicillin N + 2 H(2)O.

CC -!- COFACTOR: Iron and ascorbate.

CC -!- PATHWAY: Biosynthesis of penicillin and cephalosporin.

CC -!- SIMILARITY: Belongs to the iron/ascorbate-dependent oxidoreductase family.

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CC -----

DR EMBL; X57310; CAA40562.1; -.

DR PIR; S15284; S15284.

DR HSSP; P05326; 1BK0.

DR InterPro; IPR005123; 2OG-FeII\_Oxy.

DR InterPro; IPR002283; IPN\_synth.

DR InterPro; IPR002057; Isopen\_N\_synth.

DR Pfam; PF03171; 2OG-FeII\_Oxy; 1.

DR PRINTS; PR00682; IPNSYNTHASE.

DR PROSITE; PS00185; IPNS\_1; 1.

DR PROSITE; PS00186; IPNS\_2; FALSE\_NEG.

KW Antibiotic biosynthesis; Oxidoreductase; Iron; Vitamin C.

FT METAL 210 210 IRON (BY SIMILARITY).

FT METAL 212 212 IRON (BY SIMILARITY).

FT METAL 266 266 IRON (BY SIMILARITY).

SQ SEQUENCE 328 AA; 37466 MW; F0DE8B0727AC3855 CRC64;

Query Match 58.8%; Score 1041; DB 1; Length 328;  
Best Local Similarity 60.1%; Pred. No. 2e-81;  
Matches 196; Conservative 47; Mismatches 79; Indels 4; Gaps 3;

```
Qy      7 ANVPKIDVSPLFGDDQAAKMRVAQQIDAASRD TGFFYAVNHGINVQRLSQKTKEFHMSIT 66
      | || ||||| ||||| |:|| |:|| | | :||| | ||:||| ||| :||
Db      6 AEVPTIDVSPLFGDDAQEKVRVGQEINKACRGS GFFYAANHGVQRLQDQVNVNEFHRTMS 65

Qy     67 PEEKWDLAIRAYNKEHQDQVRAGYYLSIPGKKAVESFCYLNPNFTPDHPRIQAKTPTHEV 126
      |:||:||| |||| : || |||:|| ||||| |||||:||| ||| :| || |||
Db     66 PQEKYDLAIHAYNK--NNSHVRNGYYMAIEGKKAVESFCYLNPSFSEDHPEIKAGTPMHEV 124

Qy    127 NVWPDETKHPGFQDFAEQYYWDVFGLLSALLKGYALALGKEENFFARHFKPDDTLASVVL 186
      | |||| ||| |:|| |:||| : || |:||:|||||:||| || | |||:|||
Db    125 NSWPDEEKHPSFRPFCEEYYWTMHRLSKVLMRGFALALGKDERFFEPELKEADTLSSVSL 184

Qy    187 IRYPYLDPYPEAAIKTAADGTKLSFRWHEDVSLITVLYQSNVQNLQVETAAGYQDIEADD 246
      |||||:|| || :|| || |||| | |||:|||||:||| ||||| |:||: |
Db    185 IRYPYLEDYP--PVKTGPDGEKLSFEDHFDVSMITVLYQTQVQNLQVETVDGWRDLPTSD 242

Qy    247 TGYLINCGSYMAHLTNNYYKAPIHRVKWVNAERQSLPFFVNLGYDSVIDPFD-REPNGK 305
      | :||| |:||| |||||:|| :||:|||:||| ||||| : | ::||| | |||
Db    243 TDFLVNAGTYLGHLTNDYFPSPLHRVKFVNAERLSLPFFFFHAGQHTLIEPFFPDGAPEGK 302

Qy    306 SDREPLSYGDYLNGLVSLINKNGQT 331
      | : ||||| :|| ||| |||||
Db    303 QGNEAVRYGDYLNHGLHSLIVKNGQT 328
```



## RESULT 5

## IPNS\_STRJU

ID IPNS\_STRJU STANDARD; PRT; 329 AA.  
AC P18286;  
DT 01-NOV-1990 (Rel. 16, Created)  
DT 01-NOV-1990 (Rel. 16, Last sequence update)  
DT 10-OCT-2003 (Rel. 42, Last annotation update)  
DE Isopenicillin N synthetase (EC 1.21.3.1) (IPNS) (Isopenicillin N synthase).  
DE synthase).  
GN PCBC.  
OS Streptomyces jumonjinensis.  
OC Bacteria; Actinobacteria; Actinobacteridae; Actinomycetales;  
OC Streptomycineae; Streptomycetaceae; Streptomyces.  
OX NCBI\_TaxID=1945;  
RN [1]  
RP SEQUENCE FROM N.A.  
RX MEDLINE=89112164; PubMed=3216857;  
RA Shiffman D., Mevarech M., Jensen S.E., Cohen G., Aharonowitz Y.;  
RT "Cloning and comparative sequence analysis of the gene coding for  
RT isopenicillin N synthase in Streptomyces.";  
RL Mol. Gen. Genet. 214:562-569(1988).  
RN [2]  
RP MUTAGENESIS OF HISTIDINE AND ASPARTIC ACID RESIDUES.  
RX MEDLINE=96229923; PubMed=8639682;  
RA Borovok I., Landman O., Kreisberg-Zakarin R., Aharonowitz Y.,  
RA Cohen G.;  
RT "Ferrous active site of isopenicillin N synthase: genetic and sequence  
RT analysis of the endogenous ligands.";  
RL Biochemistry 35:1981-1987(1996).  
CC -!- FUNCTION: Removes, in the presence of oxygen, 4 hydrogen atoms  
CC from delta-L-(alpha-aminoadipyl)-L-cysteinyl-D-valine (ACV) to  
CC form the azetidinone and thiazolidine rings of isopenicillin.  
CC -!- CATALYTIC ACTIVITY: N-[(5S)-5-amino-5-carboxypentanoyl]-L-  
CC cysteinyl-D-valine + O(2) = isopenicillin N + 2 H(2)O.  
CC -!- COFACTOR: Iron and ascorbate.  
CC -!- PATHWAY: Biosynthesis of penicillin and cephalosporin.  
CC -!- SIMILARITY: Belongs to the iron/ascorbate-dependent oxidoreductase  
CC family.  
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CC -----  
DR EMBL; M36687; AAA26772.1; -.  
DR HSSP; P05326; 1BK0.  
DR InterPro; IPR005123; 2OG-FeII\_Oxy.  
DR InterPro; IPR002283; IPN\_synth.  
DR InterPro; IPR002057; Isopen\_N\_synth.  
DR Pfam; PF03171; 2OG-FeII\_Oxy; 1.  
DR PRINTS; PR00682; IPNSYNTHASE.  
DR PROSITE; PS00185; IPNS\_1; 1.  
DR PROSITE; PS00186; IPNS\_2; 1.  
KW Antibiotic biosynthesis; Oxidoreductase; Iron; Vitamin C.

FT METAL 212 212 IRON.  
 FT METAL 214 214 IRON.  
 FT METAL 268 268 IRON.  
 SQ SEQUENCE 329 AA; 37305 MW; 9C8F1EB8FB8BDFC6 CRC64;

Query Match 57.3%; Score 1014.5; DB 1; Length 329;  
 Best Local Similarity 59.4%; Pred. No. 3.7e-79;  
 Matches 193; Conservative 50; Mismatches 79; Indels 3; Gaps 2;

Qy 7 ANVPKIDVSPLFGDDQAAKMRVAQQIDAASRD TGFFYAVNHGINVQRLSQKTKEFHMSIT 66  
 | | | | | : | | | | | | | | | : | : | : | | | | | : | | | : | : |  
 Db 8 AEVPTIDISPLSGDDAKAKQ RVAQEINKAARGSGFFYASNHGVDVQLLQDVVNEFHRNMS 67  
 Qy 67 PEEKWDLAIRAYNKEHQDQVRAGYYLSIPGKKAVESFCYLNPNFTPDHPRIQAKTPTHEV 126  
 : | | | | | | | | : | | | | : | | | | | | | | | : | | | : | : | | |  
 Db 68 DQEKHDLAINAYNKDN-PHVRNGYYKAIGKKAVESFCYLNPSFSDDHPMIKSETPMHEV 126  
 Qy 127 NVWPDETKHPGFQDFAEQYYWDVFG LSSALLKGYALALGKEENFFARHFKPDDTLASVVL 186  
 | : | | | | | | | | : | | | | : | : | : | : | | | | | : | : | | | | |  
 Db 127 NLWPDEEKHPRFRPFCE DYRQLRLSTVIMRGYALALGRREDFFDEALAEADTLSSVSL 186  
 Qy 187 IRYPYLDPYPEAAIKTAADG TKLSFRWHEDVSLITVLYQSNVQNLQVETAAGYQDIEADD 246  
 | | | | | : | | : | | | | | | | | | | | : | | | | | : | | | | | | |  
 Db 187 IRYPYLEEYP--PVKTGADG TKLSFEDHLDVSMITVLYQTEVQNLQVETVDGWQDIPRSD 244  
 Qy 247 TGYLINC GSYMAHLTNNYYKAPIHRVKWVNAERQSLPFFVNLGYDSVIDPFDPREPNGKS 306  
 : | : | | | : | | : | : | : | | | | : | | | | : | : | | | : | | | |  
 Db 245 EDFLVNCGTYMGHITHDYFPAPNHRVKFINAERLSLPFFLNAGHNSVIEPFVPEGAAGTV 304  
 Qy 307 DREPLSYGDY LQNGLVSLINKNGQT 331  
 | | | : | | | : | | | | | | |  
 Db 305 KNPTTSYGEYLQHGLRALIVKNGQT 329

# RESULT 6

## IPNS\_LYSLA

ID IPNS\_LYSLA STANDARD; PRT; 326 AA.  
 AC Q48739;  
 DT 15-JUL-1999 (Rel. 38, Created)  
 DT 15-JUL-1999 (Rel. 38, Last sequence update)  
 DT 10-OCT-2003 (Rel. 42, Last annotation update)  
 DE Isopenicillin N synthetase (EC 1.21.3.1) (IPNS) (Isopenicillin N synthase).  
 GN PCBC.  
 OS Lysobacter lactamgenus.  
 OC Bacteria; Proteobacteria; Gammaproteobacteria; Xanthomonadales;  
 OC Xanthomonadaceae; Lysobacter.  
 OX NCBI\_TaxID=39596;  
 RN [1]  
 RP SEQUENCE FROM N.A.  
 RC STRAIN=YK90;  
 RX MEDLINE=96287475; PubMed=8703429;  
 RA Kimura H., Izawa M., Sumino Y.;  
 RT "Molecular analysis of the gene cluster involved in cephalosporin biosynthesis from Lysobacter lactamgenus YK90."  
 RL Appl. Microbiol. Biotechnol. 44:589-596(1996).  
 CC -!- FUNCTION: Removes, in the presence of oxygen, 4 hydrogen atoms

CC from delta-L-(alpha-aminoadipyl)-L-cysteinyl-D-valine (ACV) to  
 CC form the azetidinone and thiazolidine rings of isopenicillin.  
 CC -!- CATALYTIC ACTIVITY: N-[(5S)-5-amino-5-carboxypentanoyl]-L-  
 CC cysteinyl-D-valine + O(2) = isopenicillin N + 2 H(2)O.  
 CC -!- COFACTOR: Iron and ascorbate.  
 CC -!- PATHWAY: Biosynthesis of penicillin and cephalosporin.  
 CC -!- SIMILARITY: Belongs to the iron/ascorbate-dependent oxidoreductase  
 CC family.

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 CC -----

DR EMBL; X56660; CAA39983.1; -.  
 DR PIR; S54099; S54099.  
 DR HSSP; P05326; 1BK0.  
 DR InterPro; IPR005123; 2OG-FeII\_Oxy.  
 DR InterPro; IPR002283; IPN\_synth.  
 DR InterPro; IPR002057; Isopen\_N\_synth.  
 DR Pfam; PF03171; 2OG-FeII\_Oxy; 1.  
 DR PRINTS; PR00682; IPNSYNTHASE.  
 DR PROSITE; PS00185; IPNS\_1; 1.  
 DR PROSITE; PS00186; IPNS\_2; 1.  
 KW Antibiotic biosynthesis; Oxidoreductase; Iron; Vitamin C.  
 FT METAL 209 209 IRON (BY SIMILARITY).  
 FT METAL 211 211 IRON (BY SIMILARITY).  
 FT METAL 265 265 IRON (BY SIMILARITY).  
 SQ SEQUENCE 326 AA; 36564 MW; 25731F67173F8447 CRC64;

Query Match 56.1%; Score 993.5; DB 1; Length 326;  
 Best Local Similarity 56.7%; Pred. No. 2.2e-77;  
 Matches 185; Conservative 58; Mismatches 78; Indels 5; Gaps 4;

QY 7 ANVPKIDVSPFLFGDDQAAKMRVAQQIDAASRD TGFFYAVNHGINVQRLSQKTKEFHMSIT 66  
 Db 5 ADVPVIDISGLSGNDMDVKKDIAARIDRACRSGSFFYAANHGVDLAALQKFTTDWHMAMS 64  
 QY 67 PEEKWDLAIRAYNKEHQDQVRAGYYLSIPGKKAVESFCYLNPNFTPDHPRIQAKTPTHEV 126  
 Db 65 PEEKWELAIRAYNPAN-PRNRNGYYMAVEGKKANESFCYLNPSFDADHATIKAGLPSHEV 123  
 QY 127 NVWPDETKHPGFQDFAEQYYWDVFGFLSSALLKGYALALGKEENFFARHFKPDDTLASVVL 186  
 Db 124 NIWPDEARHPGMRRFYEAYFSDVFDVAAVILRGFAIALGREESFFERHFSMDDTLASVSL 183  
 QY 187 IRYPYLDPYPEAAIKTAADGTKLSFRWHEDVSLITVLYQSNVQNLQVETAAGYQDIEADD 246  
 Db 184 IRYPFLENYP--PLKLGPDGEKLSFEHHQDVSLITVLYQTAIPNLQVETAAGYLDIPVSD 241  
 QY 247 TGYLINCGSYMAHLTNYYKAPIHRVKWVNAERQSLPFFVNLGYDSVIDPFDPREPNKGS 306  
 Db 242 EHFLVNCGTMAHITNGYYAPVHRVKYINAERLSIPFFANLSHASAIDPFAP-PPYAPA 300

QY 307 DREP-LSYGDYLNGLVSLINKNGQT 331  
 | :|||||:|: || |||  
 Db 301 RGNPTVSYGDYLNHGLLDLIRANGQT 326

RESULT 7

IPNS\_STRCL

ID IPNS\_STRCL STANDARD; PRT; 329 AA.  
 AC P10621;  
 DT 01-JUL-1989 (Rel. 11, Created)  
 DT 01-JUL-1989 (Rel. 11, Last sequence update)  
 DT 10-OCT-2003 (Rel. 42, Last annotation update)  
 DE Isopenicillin N synthetase (EC 1.21.3.1) (IPNS) (Isopenicillin N synthase).  
 DE synthase).  
 GN PCBC.  
 OS Streptomyces clavuligerus.  
 OC Bacteria; Actinobacteria; Actinobacteridae; Actinomycetales;  
 OC Streptomycineae; Streptomyetaceae; Streptomyces.  
 OX NCBI\_TaxID=1901;  
 RN [1]  
 RP SEQUENCE FROM N.A.  
 RC STRAIN=ATCC 27064 / DSM 738 / NRRL 3585;  
 RX MEDLINE=88212175; PubMed=3130293;  
 RA Leskiw B.K., Aharonowitz Y., Mevarech M., Wolfe S., Vining L.C.,  
 RA Westlake D.W.S., Jensen S.E.;  
 RT "Cloning and nucleotide sequence determination of the isopenicillin N synthetase gene from Streptomyces clavuligerus.";  
 RT synthetase gene from Streptomyces clavuligerus.";  
 RL Gene 62:187-196(1988).  
 CC -!- FUNCTION: Removes, in the presence of oxygen, 4 hydrogen atoms  
 CC from delta-L-(alpha-aminoadipyl)-L-cysteinyl-D-valine (ACV) to  
 CC form the azetidinone and thiazolidine rings of isopenicillin.  
 CC -!- CATALYTIC ACTIVITY: N-[(5S)-5-amino-5-carboxypentanoyl]-L-  
 CC cysteinyl-D-valine + O(2) = isopenicillin N + 2 H(2)O.  
 CC -!- COFACTOR: Iron and ascorbate.  
 CC -!- PATHWAY: Biosynthesis of penicillin and cephalosporin.  
 CC -!- SIMILARITY: Belongs to the iron/ascorbate-dependent oxidoreductase  
 CC family.  
 CC -----  
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 CC -----  
 DR EMBL; M19421; AAA26770.1; -.  
 DR EMBL; A01132; CAA00131.1; -.  
 DR PIR; A29894; A29894.  
 DR HSSP; P05326; 1BLZ.  
 DR InterPro; IPR005123; 2OG-FeII\_Oxy.  
 DR InterPro; IPR002283; IPN\_synth.  
 DR InterPro; IPR002057; Isopen\_N\_synth.  
 DR Pfam; PF03171; 2OG-FeII\_Oxy; 1.  
 DR PRINTS; PR00682; IPNSYNTHASE.  
 DR PROSITE; PS00185; IPNS\_1; 1.  
 DR PROSITE; PS00186; IPNS\_2; 1.

KW Antibiotic biosynthesis; Oxidoreductase; Iron; Vitamin C.  
 FT METAL 212 212 IRON (BY SIMILARITY).  
 FT METAL 214 214 IRON (BY SIMILARITY).  
 FT METAL 268 268 IRON (BY SIMILARITY).  
 SQ SEQUENCE 329 AA; 36958 MW; 71AA1CCE9514761C CRC64;

Query Match 55.7%; Score 986.5; DB 1; Length 329;  
 Best Local Similarity 58.2%; Pred. No. 9e-77;  
 Matches 189; Conservative 52; Mismatches 81; Indels 3; Gaps 2;

Qy 7 ANVPKIDVSPLFGDDQAAKMRVAQQIDAASRD TGFFYAVNHGINVQRLSQKTKEFHMSIT 66  
 |:||| |:|:|||| | ||| |:|:| | | :|||| |:|:|:| | ||| :|  
 Db 8 AHVPTIDISPLFGTDAAAKKRVAEEIHGACRGSGFFYATNHGVDVQQLQDVVNEFHGAMT 67  
 Qy 67 PEEKWDLAIRAYNKEHQDQVRAGYYLSIPGKKAVESFCYLNPNTPDHPRIQAKTPTHEV 126  
 :|| | ||| ||| :: | | ||| :|:|:|:|:|:|:|:|:| | | | | |  
 Db 68 DQEKHDLAIHAYNPDN-PHVRNGYYKAVPGRKAVESFCYLNPDFGEDHPMIAAGTPMHEV 126  
 Qy 127 NVWPDETKHPGFQDFAEQYYWDVFLGSSALLKGYALALGKEENFFARHFKPDDTLASVVL 186  
 |:|:|:| |:| |:| | | | : |:| |:|:| | | | |:|:| |:|:| |  
 Db 127 NLWPDEERHPRFRPFCEGYRQMLKLSTVLMRGLALALGRPEHFFDAALAEQDSLSSVSL 186  
 Qy 187 IRYPYLDPYPEAAIKTAADGTKLSFRWHEDVSLITVLYQSNVQNLQVETAAGYQDIEADD 246  
 | |||||: || |:| | | | | | | |:|:|:|:|:|:| | | | | |:|:| :  
 Db 187 IRYPYLEEYP--PVKTGPDGQLLSFEDHLDVSMITVLFQTQVQNLQVETVDGWRDIPTSE 244  
 Qy 247 TGYLINCOSYMAHLTNYYKAPIHRVKWVNAERQSLPFFVNLGYDSVIDPFDPREPNGKS 306  
 :|:|:|:|:|:|:|:|:| | | | | |:|:|:|:|:|:| | |:|:| |:|:| : :  
 Db 245 NDFLVNCGTYMAHVTNDYFPAPNHRVKFVNAERLSLPFFLNGGHEAVIEPFVPEGASEEV 304  
 Qy 307 DREPLSYGDYLGQGLVSLINKNGQT 331  
 | | | | | | | |:| |:| | | | |  
 Db 305 RNEALSYGDYLGHGLRALIVKNGQT 329

# RESULT 8

## IPNS\_FLASS

ID IPNS\_FLASS STANDARD; PRT; 326 AA.  
 AC P16020;  
 DT 01-APR-1990 (Rel. 14, Created)  
 DT 01-APR-1990 (Rel. 14, Last sequence update)  
 DT 10-OCT-2003 (Rel. 42, Last annotation update)  
 DE Isopenicillin N synthetase (EC 1.21.3.1) (IPNS) (Isopenicillin N synthase).  
 DE synthase).  
 GN PCBC.  
 OS Flavobacterium sp. (strain SC 12,154).  
 OC Bacteria; Bacteroidetes; Flavobacteria; Flavobacteriales;  
 OC Flavobacteriaceae; Flavobacterium.  
 OX NCBI\_TaxID=241;  
 RN [1]  
 RP SEQUENCE FROM N.A.  
 RX MEDLINE=90174998; PubMed=2308852;  
 RA Shiffman D., Cohen G., Aharonowitz Y., von Dohren H., Kleinkauf H.,  
 RA Mevarech M.;  
 RT "Nucleotide sequence of the isopenicillin N synthase gene (pcbC) of  
 RT the Gram-negative Flavobacterium sp. SC 12,154."  
 RL Nucleic Acids Res. 18:660-660(1990).

```

CC      -!- FUNCTION: Removes, in the presence of oxygen, 4 hydrogen atoms
CC          from delta-L-(alpha-aminoadipyl)-L-cysteinyl-D-valine (ACV) to
CC          form the azetidinone and thiazolidine rings of isopenicillin.
CC      -!- CATALYTIC ACTIVITY: N-[(5S)-5-amino-5-carboxypentanoyl]-L-
CC          cysteinyl-D-valine + O(2) = isopenicillin N + 2 H(2)O.
CC      -!- COFACTOR: Iron and ascorbate.
CC      -!- PATHWAY: Biosynthesis of penicillin and cephalosporin.
CC      -!- SIMILARITY: Belongs to the iron/ascorbate-dependent oxidoreductase
CC          family.

```

```

DR      EMBL; X17355; CAA35233.1; -.
DR      HSSP; P05326; 1BK0.
DR      InterPro; IPR005123; 2OG-FeII_Oxy.
DR      InterPro; IPR002283; IPN_synth.
DR      InterPro; IPR002057; Isopen_N_synth.
DR      Pfam; PF03171; 2OG-FeII_Oxy; 1.
DR      PRINTS; PR00682; IPNSYNTHASE.
DR      PROSITE; PS00185; IPNS_1; 1.
DR      PROSITE; PS00186; IPNS_2; 1.
KW      Antibiotic biosynthesis; Oxidoreductase; Iron; Vitamin C.
FT      METAL             209      209      IRON (BY SIMILARITY).
FT      METAL             211      211      IRON (BY SIMILARITY).
FT      METAL             265      265      IRON (BY SIMILARITY).
SQ      SEQUENCE          326 AA;  36465 MW;  256E274316395837 CRC64;

```

Qy	7	ANVPKIDVSPFLFGDDQAAKMRFVAQQIDAASRDGTGFFYAVNHNHGINVQRLSQKTKEFHMSIT	66
Db	5	ADVPVIDISGLSGNDMDVKKDIAARIDRACRGSFFYAANHGVDLAALQKFTTDWHMAMS	64
Qy	67	PEEKWDLAIRAYNKEHQDQVRAGYYLSIPGKKAVESFCYLNPNFTPDHPRIQAKTPTHEV	126
Db	65	AEEKWELAIRAYNPAN-PRNRNGYYMAVEGKKANESFCYLNPSFDADHATIKAGLPSHEV	123
Qy	127	NVWPDETKHPGFQDFAEQYYWDVFLGSSALLKGYALALGKEENFFARHFKPDDTLASVVL	186
Db	124	NIWPDEARHPGMRRFYEAYFSDVFDVAAVILRGFAIALGREESFFERHFMSDDTLASVSL	183
Qy	187	IRYPYLDPYPEAAIKTAADGTKLSFRWHEDVSLITVLYQSNVQNQLQVETAAGYQDIEADD	246
Db	184	IRYPFLENYP--PLKLGPDGEKLSFEHHQDVSLITVLYQTAIPNLQVETAEGYLDIPVSD	241
Qy	247	TGYLINCGSYMAHLTNYYKAPIHRVKWVNAERQSLPFFVNLGYSVIDPFPDPREPNGKS	306
Db	242	EHFLVNCGYTMAHITNGYYAPVHRVKYINAERLSIPFFANLSHASAIDPFPAPPYAPPG	301

QY 307 DREPLSYGDYLONGLVSLINKNGQT 331  
 :|||||:|: || |||  
 Db 302 GNPTVSYGDYLGHLDDLIRANGQT 326

RESULT 9

IPNS\_STRGR

ID IPNS\_STRGR STANDARD; PRT; 329 AA.  
 AC Q54243;  
 DT 15-JUL-1999 (Rel. 38, Created)  
 DT 15-JUL-1999 (Rel. 38, Last sequence update)  
 DT 10-OCT-2003 (Rel. 42, Last annotation update)  
 DE Isopenicillin N synthetase (EC 1.21.3.1) (IPNS) (Isopenicillin N synthase).  
 GN PCBC.  
 OS Streptomyces griseus.  
 OC Bacteria; Actinobacteria; Actinobacteridae; Actinomycetales;  
 OC Streptomycineae; Streptomycetaceae; Streptomyces.  
 OX NCBI\_TaxID=1911;  
 RN [1]  
 RP SEQUENCE FROM N.A.  
 RC STRAIN=NRRL 3851;  
 RX MEDLINE=91197089; PubMed=1901702;  
 RA Garcia-Dominguea M., Liras P., Martin J.F.;  
 RT "Cloning and characterization of the isopenicillin N synthase gene of  
 RT Streptomyces griseus NRRL 3851 and studies of expression and  
 RT complementation of the cephamycin pathway in Streptomyces  
 RT clavuligerus.";  
 RL Antimicrob. Agents Chemother. 35:44-52(1991).  
 CC -!- FUNCTION: Removes, in the presence of oxygen, 4 hydrogen atoms  
 CC from delta-L-(alpha-aminoadipyl)-L-cysteinyl-D-valine (ACV) to  
 CC form the azetidinone and thiazolidine rings of isopenicillin.  
 CC -!- CATALYTIC ACTIVITY: N-[(5S)-5-amino-5-carboxypentanoyl]-L-  
 CC cysteinyl-D-valine + O(2) = isopenicillin N + 2 H(2)O.  
 CC -!- COFACTOR: Iron and ascorbate.  
 CC -!- PATHWAY: Biosynthesis of penicillin and cephalosporin.  
 CC -!- SIMILARITY: Belongs to the iron/ascorbate-dependent oxidoreductase  
 CC family.  
 CC -----  
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 CC -----  
 DR EMBL; X54609; CAA38431.1; -.  
 DR PIR; A61155; A61155.  
 DR HSSP; P05326; 1BK0.  
 DR InterPro; IPR005123; 2OG-FeII\_Oxy.  
 DR InterPro; IPR002283; IPN\_synth.  
 DR InterPro; IPR002057; Isopen\_N\_synth.  
 DR Pfam; PF03171; 2OG-FeII\_Oxy; 1.  
 DR PRINTS; PR00682; IPNSYNTHASE.  
 DR PROSITE; PS00185; IPNS\_1; 1.  
 DR PROSITE; PS00186; IPNS\_2; 1.

KW	Antibiotic biosynthesis; Oxidoreductase; Iron; Vitamin C.			
FT	METAL	212	212	IRON (BY SIMILARITY).
FT	METAL	214	214	IRON (BY SIMILARITY).
FT	METAL	268	268	IRON (BY SIMILARITY).
SQ	SEQUENCE	329 AA;	37368 MW;	0CD96C8F7CF5A7EB CRC64;

Query Match 55.6%; Score 985.5; DB 1; Length 329;  
Best Local Similarity 56.9%; Pred. No. 1.1e-76;  
Matches 185; Conservative 55; Mismatches 82; Indels 3; Gaps 2;

Qy	7	ANVPKIDVSPFLGDDQAAKMRVAQQIDAASRDTGFFYAVNHGINVQRLSQKTKEFHMSIT	66
		:     :             :     :     :	
Db	8	AHVPTIDISPLSGGDADDKRVAQEINKACRESGFFYASHHGIDVQLLKDVVNEFHRTMT	67
Qy	67	PEEKWDLAIRAYNKEHQDQVRAGYYLSIPGKKAVESFCYLNPNTPDHPRIQAKTPTHEV	126
		:   :	
Db	68	DEEKYDLAINAYNK--NNPRTNRNGYYMAVKGKKAVESWCYLNPSFSEDHPQIRSGTPMHEG	126
Qy	127	NVWPDETKHPGFQDFAEQYYWDVFGSLSSALLKGYALALGKEENFFARHFKPDDTLASVVL	186
		:	
Db	127	NIWPDEKRHRQFRPFCEQYYRDVFSLSKVLMRGFALALGKPEDFFDASLSLADTLASVTL	186
Qy	187	IRYPYLDPYPEAAIKTAADGTKLSFRWHEDVSLITVLYQSNVQNLQVETAAGYQDIEADD	246
		:	
Db	187	IHYPYLEDYP--PVKTGPDGTKLSFEDHLDVSMITVLFQTEVQNLQVETADGWQDLPTSG	244
Qy	247	TGYLINCGSYMAHLTNYYKAPIHRVKWVNAERQSLPFFVNLGYDSVIDPFDPREPNGKS	306
		:  :   :	
Db	245	ENFLVNCGYTMYGLTNDYFPAPNHRVKFINAERLSLPFFLHAGHTTVMEFPSPEDTRGKE	304
Qy	307	DREPLSYGDYLLQNGLVSLINKNGQT	331
		:	
Db	305	LNPPVRYGDYLLQOASNALIAKNGOT	329

```

RESULT 10
IPNS_STRLP
ID      IPNS_STRLP      STANDARD;          PRT;    333 AA.
AC      P12438;
DT      01-OCT-1989 (Rel. 12, Created)
DT      01-OCT-1989 (Rel. 12, Last sequence update)
DT      10-OCT-2003 (Rel. 42, Last annotation update)
DE      Isopenicillin N synthetase (EC 1.21.3.1) (IPNS) (Isopenicillin N
DE      synthase).
GN      PCBC.
OS      Streptomyces lipmanii (Streptomyces alboniger).
OC      Bacteria; Actinobacteria; Actinobacteridae; Actinomycetales;
OC      Streptomycineae; Streptomycetaceae; Streptomyces.
OX      NCBI_TaxID=132472;
RN      [1]
RP      SEQUENCE FROM N.A.
RX      MEDLINE=88314868; PubMed=3045077;
RA      Weigel B.J., Burgett S.G., Chen V.J., Skatrud P.L., Frolik C.A.,
RA      Queener S.W., Ingolia T.D.;
RT      "Cloning and expression in Escherichia coli of isopenicillin N
RT      synthetase genes from Streptomyces lipmanii and Aspergillus
RT      nidulans.";
```



RL J. Bacteriol. 170:3817-3826(1988).  
 CC -!- FUNCTION: Removes, in the presence of oxygen, 4 hydrogen atoms  
 CC from delta-L-(alpha-aminoadipyl)-L-cysteinyl-D-valine (ACV) to  
 CC form the azetidinone and thiazolidine rings of isopenicillin.  
 CC -!- CATALYTIC ACTIVITY: N-[(5S)-5-amino-5-carboxypentanoyl]-L-  
 CC cysteinyl-D-valine + O(2) = isopenicillin N + 2 H(2)O.  
 CC -!- COFACTOR: Iron and ascorbate.  
 CC -!- PATHWAY: Biosynthesis of penicillin and cephalosporin.  
 CC -!- SIMILARITY: Belongs to the iron/ascorbate-dependent oxidoreductase  
 CC family.

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 CC -----

DR EMBL; M22081; AAA26771.1; -.  
 DR HSSP; P05326; 1BK0.  
 DR InterPro; IPR005123; 2OG-FeII\_Oxy.  
 DR InterPro; IPR002283; IPN\_synth.  
 DR InterPro; IPR002057; Isopen\_N\_synth.  
 DR Pfam; PF03171; 2OG-FeII\_Oxy; 1.  
 DR PRINTS; PR00682; IPNSYNTHASE.  
 DR PROSITE; PS00185; IPNS\_1; 1.  
 DR PROSITE; PS00186; IPNS\_2; 1.  
 KW Antibiotic biosynthesis; Oxidoreductase; Iron; Vitamin C.  
 FT METAL 216 216 IRON (BY SIMILARITY).  
 FT METAL 218 218 IRON (BY SIMILARITY).  
 FT METAL 272 272 IRON (BY SIMILARITY).  
 SQ SEQUENCE 333 AA; 38082 MW; D55385664EA2CA26 CRC64;

Query Match 55.4%; Score 980.5; DB 1; Length 333;  
 Best Local Similarity 57.8%; Pred. No. 3e-76;  
 Matches 189; Conservative 50; Mismatches 85; Indels 3; Gaps 3;

Qy	7	ANVPKIDVSP	LF	GDDQAAKMR	VAQQIDAAS	RD	TGFF	YAVNHGIN	VQRL	SQKTKEFH	MSIT	66
		:		:				:		:		:
Db	8	ADVPTIDIS	PLFG	TD	PD	AKAHVARQ	INEACR	SGSGFF	YASHHG	IDVRRL	QDVVNE	FHRTMT
			:		:		:		:		:	:
Qy	67	PEEKWDLA	IRAYNKE	HQDQVR	AGYYLS	IPGKKA	VE	FCYLNPN	FTPDHP	RIQAKTP	THEV	126
		:					:		:		:	:
Db	68	DQEKHDLA	IHAYN-	ENNSHVR	NGYYMA	RPGRKT	VE	SWCYLN	PSFGED	HPMIKAG	TPMHEV	126
			:		:		:		:		:	:
Qy	127	NVWPDE	TKHPGF	QDFAE	QYYWDV	FGLSSA	-LLKGY	ALALGKE	ENFFAR	HFKPDD	TLA-SV	184
					:		:		:		:	:
Db	127	NVWPDE	ERHPDF	RSFGE	QYYREV	RLSKVLL	LRGFAL	ALGKPE	EFFENE	VTEEDT	LS	186
			:		:		:		:		:	:
Qy	185	VLIRYPY	LD	PEEAAIK	TAA	DKT	LSFR	WHEDV	SLITV	LYQSNV	QNLQV	ETAAGYQDIEA
		:										:
Db	187	LMIRYPY	LD	PEEAAIK	TGPD	GT	RLS	FEDH	LDVSM	ITVLFQ	TEVQNL	QVETVDGWQSLPT
			:		:		:		:		:	:
Qy	245	DDTGYL	INCGS	YMAHL	TNNYYK	APIHRV	KWNA	ERQSLP	FFVNLG	YDSVID	PFDP	PREPNG
		:			:		:		:		:	:
Db	247	SGENFL	INCGT	YL	GLTND	YFPAPN	HRVKY	VNAERL	SLPFFL	HAGQNS	VMPKPF	HPEDTGD
			:		:		:		:		:	:

QY 305 KSDREPLSYGDYLNQGLVSLINKNGQT 331  
 : :||:|||| | :|| || ||  
 Db 307 RKLNPVATYGEYLQEGFHAIKKNVQT 333

RESULT 11

IPNS\_STRCT

ID IPNS\_STRCT STANDARD; PRT; 321 AA.  
 AC Q53932;  
 DT 15-JUL-1999 (Rel. 38, Created)  
 DT 15-JUL-1999 (Rel. 38, Last sequence update)  
 DT 10-OCT-2003 (Rel. 42, Last annotation update)  
 DE Isopenicillin N synthetase (EC 1.21.3.1) (IPNS) (Isopenicillin N  
 DE synthase).  
 GN PCBC OR IPNS.  
 OS Streptomyces cattleya.  
 OC Bacteria; Actinobacteria; Actinobacteridae; Actinomycetales;  
 OC Streptomycineae; Streptomycetaceae; Streptomyces.  
 OX NCBI\_TaxID=29303;  
 RN [1]  
 RP SEQUENCE FROM N.A.  
 RX MEDLINE=97350503; PubMed=9206271;  
 RA Wang Y., Li R.;  
 RT "Cloning and sequencing the isopenicillin N synthetase (IPNS) gene  
 RT from Streptomyces cattleya.";  
 RL Acta Microbiol. Sin. 36:87-92(1996).  
 CC -!- FUNCTION: Removes, in the presence of oxygen, 4 hydrogen atoms  
 CC from delta-L-(alpha-aminoadipyl)-L-cysteinyl-D-valine (ACV) to  
 CC form the azetidinone and thiazolidine rings of isopenicillin.  
 CC -!- CATALYTIC ACTIVITY: N-[(5S)-5-amino-5-carboxypentanoyl]-L-  
 CC cysteinyl-D-valine + O(2) = isopenicillin N + 2 H(2)O.  
 CC -!- COFACTOR: Iron and ascorbate.  
 CC -!- PATHWAY: Biosynthesis of penicillin and cephalosporin.  
 CC -!- SIMILARITY: Belongs to the iron/ascorbate-dependent oxidoreductase  
 CC family.  
 CC -----  
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 CC -----  
 DR EMBL; D78166; BAA11234.1; -.  
 DR PIR; A58458; A58458.  
 DR HSSP; P05326; 1BK0.  
 DR InterPro; IPR005123; 2OG-FeII\_Oxy.  
 DR InterPro; IPR002283; IPN\_synth.  
 DR InterPro; IPR002057; Isopen\_N\_synth.  
 DR Pfam; PF03171; 2OG-FeII\_Oxy; 1.  
 DR PRINTS; PR00682; IPNSYNTHASE.  
 DR PROSITE; PS00185; IPNS\_1; 1.  
 DR PROSITE; PS00186; IPNS\_2; 1.  
 KW Antibiotic biosynthesis; Oxidoreductase; Iron; Vitamin C.  
 FT METAL 213 213 IRON (BY SIMILARITY).

Query Match 41.7%; Score 738.5; DB 1; Length 321;  
Best Local Similarity 48.3%; Pred. No. 1.3e-55;  
Matches 152; Conservative 54; Mismatches 104; Indels 5; Gaps 5;

```

RESULT 12
FLS_MATIN
ID   FLS_MATIN          STANDARD;          PRT;    291 AA.
AC   004395;
DT   15-JUL-1999 (Rel. 38, Created)
DT   15-JUL-1999 (Rel. 38, Last sequence update)
DT   10-OCT-2003 (Rel. 42, Last annotation update)
DE   Flavonol synthase (EC 1.14.11.-) (FLS) (Fragment).
OS   Matthiola incana (Common stock).
OC   Eukaryota; Viridiplantae; Streptophyta; Embryophyta; Tracheophyta;
OC   Spermatophyta; Magnoliophyta; eudicotyledons; core eudicots; rosids;
OC   eurosids II; Brassicales; Brassicaceae; Matthiola.
OX   NCBI_TaxID=3724;
RN   [1]
RP   SEQUENCE FROM N.A.
RC   TISSUE=Flower buds, and Petal;
RA   Henkel J., Forkmann G.;
RT   "Cloning and expression of a flavonol synthase gene from common
RT   stock (Matthiola incana).";
RL   Submitted (APR-1997) to the EMBL/GenBank/DDBJ databases.
CC   -!- FUNCTION: Catalyzes the formation of flavonols from
CC   dihydroflavonols. It can act on dihydrokaempferol to produce
CC   kaempferol, on dihydroquercetin to produce quercetin and on
CC   dihydromyricetin to produce myricetin.

```

CC -!- COFACTOR: Iron and ascorbate.  
 CC -!- PATHWAY: Part of the biosynthetic pathway for flavonols which are  
 CC flavonoids. Flavonols are important co-pigments in flower or fruit  
 CC color and are also essential for pollen tube growth.  
 CC -!- SUBCELLULAR LOCATION: Cytoplasmic.  
 CC -!- SIMILARITY: Belongs to the iron/ascorbate-dependent oxidoreductase  
 CC family.

CC -----  
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 CC -----

DR EMBL; AF001391; AAB58800.1; -.  
 DR InterPro; IPR005123; 2OG-FeII\_Oxy.  
 DR Pfam; PF03171; 2OG-FeII\_Oxy; 1.  
 KW Flavonoid biosynthesis; Oxidoreductase; Dioxxygenase; Iron; Vitamin C.  
 FT NON\_TER 1 1  
 SQ SEQUENCE 291 AA; 33430 MW; 6B8E4E3D2834720A CRC64;

Query Match 12.3%; Score 218; DB 1; Length 291;  
 Best Local Similarity 26.1%; Pred. No. 2.9e-11;  
 Matches 91; Conservative 50; Mismatches 120; Indels 88; Gaps 18;

Qy 9 VPKIDVSPFLFGDDQAAMRVAQQIDAASRD TGFFYAVNHGIN--VQRLSQKTKEFHMSI 65  
 || :||| |:: ||: | || | | ||||| :||| : ||| :  
 Db 2 VPVVDLS--CPDEEL---VARTVVKASEDWGVFQVVNHGIPTELIQRLQKVGREF-FEL 54  
 Qy 66 TPEEKWDLAIRAYNKEHQDQVRAGY---YLSIPGKKAVESFCYLNPNFTPDHPRIQAKT 121  
 || | | : | || | | : | : || :  
 Db 55 PEA EKRS CAREAGSVE-----GYGRRIELDIKKRKGIVDQIYL-----STW 95  
 Qy 122 PTHEVN--VWPDETKHPGFQDFAEQYYWDV FGLSSALLKGYALALG-----KEEN---- 169  
 | || || | : : | : | || : : : || ||  
 Db 96 PPSSVNYRYWPKSP--PDYREVNEEYARHVKT LSEKIMEWLSEGLGLGREAIKEVNGCWY 153  
 Qy 170 -FFARHFKPDDTLASVVLIRYPYLDPYPEAAIKTAADGTKLSFRWHEDVSLITVLYQSNV 228  
 | : | ||: | : | | : : | : : :  
 Db 154 VMNINHYP-----YPHSDSFN-----GLEPHTDINGLTLITNEI 189  
 Qy 229 QNLQVETAAGYQDIEADDTGYLINC GSYMAHLTNYYKAPIHRVKWVNAE--RQSLPFFV 286  
 ||| : : : | : : | : | : | : | : | :  
 Db 190 PGLQVFKDDHWIEVEYIPSAIIVNIGDQIMMLSNGKYKNVLHKTT-VDKEKTRMSWPVLV 248  
 Qy 287 NLGYDSVIDPF-----DPREPNGKSDREPLSYGDYLQNGLVSLINKN 328  
 : || | : | || | | : : | : | : | :  
 Db 249 SPTYDMVVGPLPELTSEDDP--PKFK----PIAYKDYVHNKITFLKNKS 291

RESULT 13  
 ISP7\_SCHPO  
 ID ISP7\_SCHPO STANDARD; PRT; 397 AA.  
 AC P40902;  
 DT 01-FEB-1995 (Rel. 31, Created)

DT 01-FEB-1995 (Rel. 31, Last sequence update)  
 DT 10-OCT-2003 (Rel. 42, Last annotation update)  
 DE Sexual differentiation process protein isp7.  
 GN ISP7 OR SPAC25B8.13C.  
 OS Schizosaccharomyces pombe (Fission yeast).  
 OC Eukaryota; Fungi; Ascomycota; Schizosaccharomycetes;  
 OC Schizosaccharomycetales; Schizosaccharomycetaceae;  
 OC Schizosaccharomyces.  
 OX NCBI\_TaxID=4896;  
 RN [1]  
 RP SEQUENCE FROM N.A.  
 RX MEDLINE=95042833; PubMed=7954893;  
 RA Sato S., Suzuki H., Widyastuti U., Hotta Y., Tabata S.;  
 RT "Identification and characterization of genes induced during sexual  
 RT differentiation in Schizosaccharomyces pombe.";  
 RL Curr. Genet. 26:31-37(1994).  
 RN [2]  
 RP SEQUENCE FROM N.A.  
 RC STRAIN=972;  
 RX MEDLINE=21848401; PubMed=11859360;  
 RA Wood V., Gwilliam R., Rajandream M.A., Lyne M., Lyne R., Stewart A.,  
 RA Sgouros J., Peat N., Hayles J., Baker S., Basham D., Bowman S.,  
 RA Brooks K., Brown D., Brown S., Chillingworth T., Churcher C.M.,  
 RA Collins M., Connor R., Cronin A., Davis P., Feltwell T., Fraser A.,  
 RA Gentles S., Goble A., Hamlin N., Harris D., Hidalgo J., Hodgson G.,  
 RA Holroyd S., Hornsby T., Howarth S., Huckle E.J., Hunt S., Jagels K.,  
 RA James K., Jones L., Jones M., Leather S., McDonald S., McLean J.,  
 RA Mooney P., Moule S., Mungall K., Murphy L., Niblett D., Odell C.,  
 RA Oliver K., O'Neil S., Pearson D., Quail M.A., Rabinowitsch E.,  
 RA Rutherford K., Rutter S., Saunders D., Seeger K., Sharp S.,  
 RA Skelton J., Simmonds M., Squares R., Squares S., Stevens K.,  
 RA Taylor K., Taylor R.G., Tivey A., Walsh S.V., Warren T., Whitehead S.,  
 RA Woodward J., Volckaert G., Aert R., Robben J., Grymonprez B.,  
 RA Weltjens I., Vanstreels E., Rieger M., Schaefer M., Mueller-Auer S.,  
 RA Gabel C., Fuchs M., Fritzc C., Holzer E., Moestl D., Hilbert H.,  
 RA Borzym K., Langer I., Beck A., Lehrach H., Reinhardt R., Pohl T.M.,  
 RA Eger P., Zimmermann W., Wedler H., Wambutt R., Purnelle B.,  
 RA Goffeau A., Cadieu E., Dreano S., Gloux S., Lelaure V., Mottier S.,  
 RA Galibert F., Aves S.J., Xiang Z., Hunt C., Moore K., Hurst S.M.,  
 RA Lucas M., Rochet M., Gaillardin C., Tallada V.A., Garzon A., Thode G.,  
 RA Daga R.R., Cruzado L., Jimenez J., Sanchez M., del Rey F., Benito J.,  
 RA Dominguez A., Revuelta J.L., Moreno S., Armstrong J., Forsburg S.L.,  
 RA Cerrutti L., Lowe T., McCombie W.R., Paulsen I., Potashkin J.,  
 RA Shpakovski G.V., Ussery D., Barrell B.G., Nurse P.;  
 RT "The genome sequence of Schizosaccharomyces pombe.";  
 RL Nature 415:871-880(2002).  
 CC -!- DEVELOPMENTAL STAGE: Transcribed specifically during sexual  
 CC development.  
 CC -!- SIMILARITY: Belongs to the iron/ascorbate-dependent oxidoreductase  
 CC family.  
 CC -----  
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DR EMBL; D14064; BAA03150.1; -.

DR EMBL; AL133225; CAB61779.1; -.

DR PIR; S45496; S45496.

DR GeneDB\_SPombe; SPAC25B8.13c; -.

DR InterPro; IPR005123; 2OG-FeII\_Oxy.

DR Pfam; PF03171; 2OG-FeII\_Oxy; 1.

KW Oxidoreductase; Iron; Vitamin C.

SQ SEQUENCE 397 AA; 43810 MW; 5076C03C39B10A2B CRC64;

Query Match 12.3%; Score 218; DB 1; Length 397;  
 Best Local Similarity 21.9%; Pred. No. 4.4e-11;  
 Matches 86; Conservative 56; Mismatches 134; Indels 116; Gaps 14;

QY	9	VPKIDVSPLFGDDQAAKMRVAQQIDAASRD TGFFYAVNHGIN---VQRLSQKTKEFHMSI	65
		:       :   :  :          : : :  : :	
Db	25	MPLIDFGPYVNQEPGAHERIIQQLRAACESTGFFQIVNSPISPDVVKNAPFRASKQF-FEL	83
QY	66	TPEEKWDLAIRAYNKEHQD-----QVRAGYYLSIPGKKAV---	100
		:     : : : :         : :	
Db	84	PFDEKLTLSKDMFSNRGYELMEDFVLEGEEDSSSPLEISGIDFEAGSY---PGEAPLPPS	140
QY	101	-----ESFCYLNPNTPTDHPRIQ	118
		:     :   :	
Db	141	SIGYVLPSSSLANGEGSSMFDADMTTSNAVAHGDESI NEFRESFYFGNDNLSKD----	196
QY	119	AKTPTHEVNVWPDETKHPGFQDFAEQYYWDV FGLSSALLKGYALALGKEENFFARHFKPD	178
		: : : : : : :   :	
Db	197	LLRPFQGPKNKP-STAGSSFRKALVKYHDQMLAFANHVM SLLAESL-----ELSPD	246
QY	179	-----DTLASVVLIRYPYLDPYPEAAIKTAADG TKLSFRWHEDVSLITVLYQSNVQNL	231
		: :     : :   :   :  :  :	
Db	247	AFDEFCSDP TTSIRLLRYP-----SSPNRLGVQEHTDADAL TLMSQDNVKGL	293
QY	232	QV--ETAAGYQDIEADDTGYLINC GSYMAHLTNNYYKAPIHRV-KWVNAERQSLPFFVNL	288
		: : : : :                  :     : :      :	
Db	294	EILDVPSNCF LSVSPAPGALIANLGDIMAILTNNRYKSSMHRVCNNSGSDRYTIPFFLQG	353
QY	289	GYDSVIDPFDPREPN-GKSDREPLSYGDY LQN	319
		:            : :     :	
Db	354	NIDYVVAPL----PGLGPSTAEP IAVEDLLRD	381

# RESULT 14

## FLS\_SOLTU

ID FLS\_SOLTU STANDARD; PRT; 349 AA.

AC Q41452;

DT 01-NOV-1997 (Rel. 35, Created)

DT 01-NOV-1997 (Rel. 35, Last sequence update)

DT 10-OCT-2003 (Rel. 42, Last annotation update)

DE Flavonol synthase (EC 1.14.11.-) (FLS).

OS Solanum tuberosum (Potato).

OC Eukaryota; Viridiplantae; Streptophyta; Embryophyta; Tracheophyta;

OC Spermatophyta; Magnoliophyta; eudicotyledons; core eudicots; asterids;

OC lamiids; Solanales; Solanaceae; Solanum.

OX NCBI\_TaxID=4113;

RN [1]  
 RP SEQUENCE FROM N.A.  
 RC TISSUE=Pistil;  
 RX MEDLINE=97177800; PubMed=9025306;  
 RA van Eldik G.J., Ruiter R.K., Reijnen W.H., van Herpen M.M.A.,  
 RA Schrauwen J.A.M., Wullems G.J.;  
 RT "Regulation of flavonol biosynthesis during anther and pistil  
 RT development, and during pollen tube growth in Solanum tuberosum.";  
 RL Plant J. 11:105-113(1997).  
 CC -!- FUNCTION: Catalyzes the formation of flavonols from  
 CC dihydroflavonols. It can act on dihydrokaempferol to produce  
 CC kaempferol, on dihydroquercetin to produce quercetin and on  
 CC dihydromyricetin to produce myricetin.  
 CC -!- COFACTOR: Iron and ascorbate (By similarity).  
 CC -!- PATHWAY: Part of the biosynthetic pathway for flavonols which are  
 CC flavonoids. Flavonols are important co-pigments in flower or fruit  
 CC color and are also essential for pollen tube growth.  
 CC -!- SUBCELLULAR LOCATION: Cytoplasmic.  
 CC -!- DEVELOPMENTAL STAGE: Temporally expressed during flower  
 CC development.  
 CC -!- SIMILARITY: Belongs to the iron/ascorbate-dependent oxidoreductase  
 CC family.  
 CC -----  
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 CC -----  
 DR EMBL; X92178; CAA63092.1; -.  
 DR PIR; T07373; T07373.  
 DR InterPro; IPR005123; 2OG-FeII\_Oxy.  
 DR Pfam; PF03171; 2OG-FeII\_Oxy; 1.  
 KW Flavonoid biosynthesis; Oxidoreductase; Dioxygenase; Iron; Vitamin C.  
 SQ SEQUENCE 349 AA; 39728 MW; ADBBC3F6B10A0E05 CRC64;

Query Match 10.9%; Score 192.5; DB 1; Length 349;  
 Best Local Similarity 25.2%; Pred. No. 5.5e-09;  
 Matches 82; Conservative 52; Mismatches 134; Indels 57; Gaps 15;

Qy 9 VPKIDVSPFLFGDDQAAKMRVAQQIDAASRDTGFFYAVNHGIN---VQRLSQKTKEFHMSI 65  
 || ||:| : |:: :: ||:| | :||| :: | : ||| :  
 Db 57 VPVIDISNVDDDEE---KLVKEIVEASKEWGIFQVINHGIPDEVLENLQKVGKEFFEEV 112  
 Qy 66 TPEEKWDLAIRAYNKEHQDQVRAGYYLS----IPGKKAVESFCYLNPNFTPDHPRIQAKT 121  
 ||| :| :| | | | | ||| ||  
 Db 113 PQEEKELIA-----KKPGAQSLEGYGTSLQKEIEGKKG-----WVDH-LFHKIW 155  
 Qy 122 PTHEVN--VWPDETKHPGFQDFAEQYYWDVFLSSALLKGYALALGKEENFFARHFKPDD 179  
 | :| || |:: |:| : :: : : | || | : |  
 Db 156 PPSAINRYRWPKNP--PSYREANEYAKWLRKVADGIFRSLSLGLGLEGHEMMEAAGSED 213  
 Qy 180 TLASVVLIRYPYLDPYPEAAIKTAADGTKLSFRWHEDVSLITVLYQSNVQNLQVETAAGY 239  
 : : : || | :| : | | :| ||| : | || :  
 Db 214 IVYMLKINYPPC-PRPDLAGVVA-----HTDMSYITLLVPNEV---QVFKDGHW 260

QY 240 QDIEADDTGYLINCGSYMAHLTNYYKAPIHRVKWVN--AERQSLPFFVNLGYDSVIDPF 297  
 | : : : | : | : | : | : | : : : |  
 Db 261 YDVNYIPNAIIVHIGDQVEILSNGKYKSVYHRTT-VNKYKTRMSWPVFLEPSSEHEVGPI 319  
 QY 298 DPREPNGKSDREP-----LSYGDYL 317  
 | : : : | : | : | : | : | : : : |  
 Db 320 ----PNLINEANPPKFKTKKYKD YV 340

# RESULT 15

## FLS\_EUSGR

ID FLS\_EUSGR STANDARD; PRT; 334 AA.  
 AC Q9M547;  
 DT 16-OCT-2001 (Rel. 40, Created)  
 DT 16-OCT-2001 (Rel. 40, Last sequence update)  
 DT 10-OCT-2003 (Rel. 42, Last annotation update)  
 DE Flavonol synthase (EC 1.14.11.-) (FLS).  
 GN FLS.  
 OS Eustoma grandiflorum (Bluebells) (Lisianthus russellianus).  
 OC Eukaryota; Viridiplantae; Streptophyta; Embryophyta; Tracheophyta;  
 OC Spermatophyta; Magnoliophyta; eudicotyledons; core eudicots; asterids;  
 OC lamiids; Gentianales; Gentianaceae; Eustoma.  
 OX NCBI\_TaxID=52518;  
 RN [1]  
 RP SEQUENCE FROM N.A.  
 RA Nielsen K.M.;  
 RT "cDNA cloning of flavonol synthase and antisense suppression of  
 RT expression in *Lisianthus grandiflorum* grise.";  
 RL Submitted (MAR-2000) to the EMBL/GenBank/DDBJ databases.  
 CC -!- FUNCTION: Catalyzes the formation of flavonols from  
 CC dihydroflavonols. It can act on dihydrokaempferol to produce  
 CC kaempferol, on dihydroquercetin to produce quercetin and on  
 CC dihydromyricetin to produce myricetin (By similarity).  
 CC -!- COFACTOR: Iron and ascorbate (By similarity).  
 CC -!- PATHWAY: Part of the biosynthetic pathway for flavonols which are  
 CC flavonoids. Flavonols are important co-pigments in flower or fruit  
 CC color and are also essential for pollen tube growth.  
 CC -!- SUBCELLULAR LOCATION: Cytoplasmic (By similarity).  
 CC -!- SIMILARITY: Belongs to the iron/ascorbate-dependent oxidoreductase  
 CC family.  
 CC -----  
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 CC -----  
 DR EMBL; AF240764; AAF64168.1; -.  
 DR InterPro; IPR005123; 2OG-FeII\_Oxy.  
 DR Pfam; PF03171; 2OG-FeII\_Oxy; 1.  
 KW Flavonoid biosynthesis; Oxidoreductase; Dioxygenase; Iron; Vitamin C.  
 SQ SEQUENCE 334 AA; 38080 MW; 4097830ABE2534E2 CRC64;

Query Match 10.7%; Score 189; DB 1; Length 334;



Best Local Similarity 24.8%; Pred. No. 1e-08;  
Matches 82; Conservative 45; Mismatches 133; Indels 70; Gaps 13;

```
Qy      9 VPKIDVSPLFGDDQAAKMRVAQQIDAASRDGFFYAVNHGIN--VQRLSQKTKEFHMSI 65
      || ||:|      : : ::      : ||:: | | |||||      ::| : | | :
Db      43 VPVIDLS-----DSDEKKIVGLVSEASKEWGIFQVNVHGIPNEVIRKLQEVGKHF-FEL 95

Qy      66 TPEEKWDLAIRAYNKEHQDQVRAGY----YLSIPGKKAVESFCY-----LNPNFTPD 113
      ||| :|      |      | ||      : |||      :      :| | |
Db      96 PQEEKELIA-----KPEGSQSIEGYGTRLQKEVDGKKGWVDHLFHKIWPPSAINYQFWPK 150

Qy     114 HPRIQAKTPTHEVNVWPDETKHPGFQDFAEQYYWDVFGLSALLKGYALALGKEENFFAR 173
      :|      | ::| :| : : | | :| | | |
Db     151 NP-----PAYREANEYYAKRLQLVVDNLFKYLSLGLDLEPNSFKD 190

Qy     174 HFKPDDTLASVVLIRYPYLDPYPEAAIKTAADGTKLSFRWHEDVSLITVLYQSNVQNLQV 233
      || : : : || | :| : |      | :| ||| : | |||
Db     191 GAGGDDLVLMLKINYPPC-PRPDLAGVA-----HTDMSAITVLPNEVPGLQV 239

Qy     234 ETAAGYQDIEADDTGYLINCOSYMAHLTNYYKAPIHRVKWVNAE--RQSLPFFVNLGYD 291
      : | :      ::| : : :| ||: || | | | | : |
Db     240 YKDGHWYDCKYIPNALIVHIGDQVEIMSNGKYKSVYHRTT-VNKEKTRMSWPVFLEPPD 298

Qy     292 SVIDPFDPREPNGKSDREPL-----SYGDY 316
      : |      | : : |      | ||
Db     299 HEVGPI----PKLVNEENPAKFKTKKYKDY 324
```